Electronic Transactions on Numerical Analysis
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Contents

1 A multigrid method for distributed parameter estimation problems. *U. M. Ascher and E. Haber.*

Abstract.
This paper considers problems of distributed parameter estimation from data measurements on solutions of partial differential equations (PDEs). A nonlinear least squares functional is minimized to approximately recover the sought parameter function (i.e., the model). This functional consists of a data fitting term, involving the solution of a finite volume or finite element discretization of the forward differential equation, and a Tikhonov-type regularization term, involving the discretization of a mix of model derivatives. We develop a multigrid method for the resulting constrained optimization problem. The method directly addresses the discretized PDE system which defines a critical point of the Lagrangian. The discretization is cell-based. This system is strongly coupled when the regularization parameter is small. Moreover, the compactness of the discretization scheme does not necessarily follow from compact discretizations of the forward model and of the regularization term. We therefore employ a Marquardt-type modification on coarser grids. Alternatively, fewer grids are used and a preconditioned Krylov-space method is utilized on the coarsest grid. A collective point relaxation method (weighted Jacobi or a Gauss-Seidel variant) is used for smoothing. We demonstrate the efficiency of our method on a classical model problem from hydrology.

Key Words.
distributed parameter estimation; inverse problem; multigrid method.

AMS(MOS) Subject Classifications.
65M32, 65N55.

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Forward References.

18 An additive Schwarz preconditioner for the spectral element ocean model formulation of the shallow water equations. *Craig C. Douglas, Gundolf Haase and Mohamed Iskandarani.*

Abstract.
We discretize the shallow water equations with an Adams-Bashford scheme combined with the Crank-Nicholson scheme for the time derivatives and spectral elements for the discretization in space. The resulting coupled system of equations will be reduced to a Schur complement system with a special structure of the Schur complement. This system can be solved with a preconditioned conjugate gradients, where the matrix-vector product is only implicitly given. We derive an overlapping

block preconditioner based on additive Schwarz methods for preconditioning the reduced system.

Key Words.
Shallow water equations, h-p finite elements, adaptive grids, multigrid, parallel computing, conjugate gradients, additive Schwarz preconditioner.

AMS(MOS) Subject Classifications.
68W10, 65Y05, 47N40, 76D33

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vol.15.2003/pp18-28.dir/pp18-28.ps;
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Forward References.

29 On the accuracy of multigrid truncation error estimates. *Scott R. Fulton.*

Abstract.
In solving boundary-value problems, multigrid methods can provide computable estimates of the truncation error by comparing discretizations on grids of different mesh sizes. In the standard formulation, such estimates are contaminated by errors larger than the truncation error itself unless the residual transfer operator satisfies a restrictive condition (typically valid for injection but not for full weighting) or is itself high-order accurate. This paper proves that a simple generalization based on the work of Schaffer leads to accurate truncation error estimates without these restrictions. Numerical results for several model problems illustrate the analysis.

Key Words.
multigrid, truncation error, tau extrapolation.

AMS(MOS) Subject Classifications.
65N15, 65N50, 65N55

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Forward References.

38 Efficient solution of symmetric eigenvalue problems using multigrid preconditioners in the locally optimal block conjugate gradient method. *Andrew V. Knyazev and Klaus Neymeyr.*

Abstract.
We present a short survey of multigrid–based solvers for symmetric eigenvalue problems. We concentrate our attention on "off the shelf" and "black box" methods, which should allow solving eigenvalue problems with minimal, or no, effort on the part of the developer, taking advantage of already existing algorithms and software. We consider a class of such methods, where the multigrid only appears as a black-box tool for constructing the preconditioner of the stiffness matrix, and the base iterative algorithm is one of well-known off-the-shelf preconditioned gradient methods such as the locally optimal block preconditioned conjugate gradient method. We review some known theoretical results for preconditioned gradient methods that

guarantee the optimal, with respect to the grid size, convergence speed. Finally, we present results of numerical tests, which demonstrate practical effectiveness of our approach for the locally optimal block conjugate gradient method preconditioned by the standard V-cycle multigrid applied to the stiffness matrix.

Key Words.
symmetric eigenvalue problems, multigrid preconditioning, preconditioned conjugate gradient iterative method.

AMS(MOS) Subject Classifications.
65N25,65N55,65F15.

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56 Local approximation estimators for algebraic multigrid. *Jan Mandel.*

Abstract.
In Smoothed Aggregation Algebraic Multigrid, the prolongator is defined by smoothing of the output of a simpler tentative prolongator. The weak approximation property for the tentative prolongator is known to give a bound on the convergence factor of the two-level and even multilevel method. It is known how to bound the constants in the weak approximation property when the system matrix is given as the sum of positive semidefinite local matrices. In practice, however, the local matrices are often not known to the solver, or the problem is given in terms of local matrices and additional constraints. We characterize the matrices that can be decomposed into a sum of local positive semidefinite matrices with only given rows and columns allowed to be nonzero, and we show that such a decomposition may not always exist. We then propose a construction of approximate local matrices that may be used for local estimates. Finally, we show how eliminating the constraints from the local matrices can be used to obtain rigorous bounds.

Key Words.
Adaptive Algebraic Multigrid, robust iterative methods, local element matrices, decomposition of global matrix, apriori convergence estimates, weak approximation property.

AMS(MOS) Subject Classifications.
65N55, 65N22, 65F10, 65N30

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vol.15.2003/pp56-65.dir/pp56-65.ps;
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Forward References.

66 Cache aware data laying for the Gauss-Seidel smoother. *Malik Silva.*

Abstract.
Feeding the processor with data operands is the bottleneck in many scientific computations. This bottleneck is alleviated by means of caches, small fast memories to

keep data. The performance of a memory-intensive computation depends critically on whether most of the data accesses can be performed within the cache. Thus, cache aware computing is of importance. There are several well established strategies available to a programmer to make a program cache friendly. In this paper, we describe cache aware data laying, a technique which we feel has not been researched sufficiently. It is a promising technique as we achieved considerable performance improvements. For example, our data laying experiments with the Gauss-Seidel smoother resulted in up to 84% execution time improvements over the parallelogram based blocked implementation of the algorithm.

Key Words.
memory barrier, caches, iterative algorithms, cache-aware algorithms, data laying.

AMS(MOS) Subject Classifications.
65, 68I

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vol.15.2003/pp66-77.dir/pp66-77.ps;
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Forward References.

78 Comparison of non-linear solvers for the solution of radiation transport equations. *Linda Stals.*

Abstract.
We compare the performance of an inexact Newton-multigrid method and Full Approximation Storage multigrid when solving radiation transport equations. We also present an adaptive refinement algorithm and explore its impact on the solution of such equations.

Key Words.
FAS, Multigrid, Newton Method, Radiation Transport.

AMS(MOS) Subject Classifications.
35K55, 65M55, 65M60, 49M15

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vol.15.2003/pp78-93.dir/pp78-93.pdf;

Forward References.

94 Multilevel preconditioners for Lagrange multipliers in domain imbedding. *Janne Martikainen, Tuomo Rossi and Jari Toivanen.*

Abstract.
A domain imbedding method where the Dirichlet boundary conditions are treated using boundary supported Lagrange multipliers is considered. The discretization leads to a saddle-point problem which is solved iteratively by using either the PMINRES method with a block-diagonal preconditioner or the PCG method in an Uzawa type approach. In both cases, the preconditioning of the Schur complement related to Lagrange multipliers is based on a special sparse implementation of BPX/MDS

method. The developed preconditioning technique is well-suited even for three-dimensional problems in domains with complicated shapes. Several numerical experiments for two-dimensional and three-dimensional problems demonstrate the efficiency and the applicability of the proposed method.

Key Words.
domain imbedding method, Lagrange multipliers, multilevel methods, preconditioning.

AMS(MOS) Subject Classifications.
65F10, 65N22, 65N55

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Forward References.

106 Advancing analysis capabilities in ANSYS through solver technology. *Gene Poole, Yong-Cheng Liu and Jan Mandel.*

Abstract.
This paper describes substantial improvements in analysis capabilities in a large scale commercial finite element program made possible by the implementation of solver technology. The ANSYS program is a commercial finite element analysis program, which has been in use for thirty years. The original code, developed around a direct frontal solver has been expanded over the years to include full featured pre- and post- processing capabilities, which support a comprehensive list of analysis capabilities including linear static analysis, multiple nonlinear analyses, modal analysis and many other analysis types. The finite element models on which these analyses are used have continued to grow in size and complexity. This growth in size and complexity has been both enabled by and dependent on new solver technology along with increased computer memory and CPU resources. Beginning in 1994, ANSYS added a Jacobi preconditioned conjugate gradient solver (JCG) and subsequently an Incomplete Cholesky Preconditioned Conjugate Gradient solver (ICCG) to improve thermal analysis capabilities. In recent years the addition of the Boeing sparse matrix library for modal and static analysis, and a proprietary preconditioned conjugate gradient solver as well as additional iterative solvers, to support new CFD capabilities have greatly increased the number of solver options available in ANSYS. Most recently, in version 5.7, ANSYS has added a new domain decomposition solver for solving very large structural analysis solutions on distributed MPI-based computer systems and the newest iterative solver option, an algebraic multi-grid iterative solver (AMG). This paper will describe implementation considerations for the addition of new solver technology to a large legacy code, compare resource requirements for the various solver choices and present some comparative results from several customer generated problems. The AMG solver benefits, both in improved robustness and parallel processing efficiency, will be described. The paper will also discuss some of the implementation challenges that have been overcome to add new solver technology to a large existing code. The role of solver technology in meeting current and future demands of large scale commercial analysis codes will be discussed.

Key Words.
Finite elements, elasticity, iterative solvers, algebraic multigrid.

AMS(MOS) Subject Classifications.
65N55, 65F10, 65N30, 65N22

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vol.15.2003/pp106-121.dir/pp106-121.ps;
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Forward References.

122 A robust and parallel multigrid method for convection diffusion equations. *Michael Bader and Christoph Zenger.*

Abstract.
We present a multigrid method for the solution of convection diffusion equations that is based on the combination of recursive substructuring techniques and the discretization on hierarchical bases and generating systems. Robustness of the resulting method, at least for a variety of benchmark problems, is achieved by a partial elimination of couplings between certain "coarse grid unknowns". The choice of these coarse grid unknowns is motivated by the physical properties of the convection diffusion equation, but it is independent of the actual discretized operator. The resulting algorithm has a memory requirement that grows linearly with the number of unknowns; likewise do the computational costs of the setup and of the individual relaxation cycles. We present numerical examples that indicate that the number of iterations needed to solve a convection diffusion equation is also substantially independent of the number of unknowns and of the type and strength of the convection field.

Key Words.
convection diffusion equation, multigrid, substructuring method, parallelization.

AMS(MOS) Subject Classifications.
65N55, 76R99, 65Y05

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Forward References.

132 A multigrid algorithm for solving the multi-group, anisotropic scattering Boltzmann equation using first-order system least-squares methodology. *B. Chang and B. Lee.*

Abstract.
This paper describes a multilevel algorithm for solving the multi-group, anisotropic scattering Boltzmann equation formulated with a first-order system least-squares methodology. A $P_n - h$ finite element discretization is used. The resulting angle discretization of this P_n approach does not exhibit the so-called "ray effects," but this discretization leads to a large coupled system of partial differential equations for the spatial coefficients, and, on scaling the system to achieve better approximation, the system coupling depends strongly on the material parameters. Away from the

thick, low absorptive regime, a relatively robust multigrid algorithm for solving these spatial systems will be described. For the thick, low absorptive regime, where an incompressible elasticity-like equation appears, an additive/multiplicative Schwarz smoother gives substantial multigrid improvement over standard nodal smoothers. Rather than using higher-order or Raviart-Thomas finite element spaces, which lead to complicated implementation, only low-order, conforming finite elements are used. Numerical examples illustrating almost $h-$independent convergence rates and locking-free discretization accuracy will be given.

Key Words.
Boltzmann transport equation, first-order system least-squares, multigrid method.

AMS(MOS) Subject Classifications.
65N30, 65N55, 65N15.

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vol.15.2003/pp132-151.dir/pp132-151.ps;
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Forward References.

152 Large-eddy simulation and multigrid methods. *Sandra Nägele and Gabriel Wittum.*

Abstract.
A method to simulate turbulent flows with Large-Eddy Simulation on unstructured grids is presented. Two kinds of dynamic models are used to model the unresolved scales of motion and are compared with each other on different grids. Thereby the behaviour of the models is shown and additionally the feature of adaptive grid refinement is investigated. Furthermore the parallelization aspect is addressed.

Key Words.
LES, turbulence, multigrid, parallelization.

AMS(MOS) Subject Classifications.
65N55, 65Y05, 76F65

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Forward References.

165 On multigrid for linear complementarity problems with application to American-style options. *C. W. Oosterlee.*

Abstract.
We discuss a nonlinear multigrid method for a linear complementarity problem. The convergence is improved by a recombination of iterants. The problem under consideration deals with option pricing from mathematical finance. Linear complementarity problems arise from so-called American-style options. A 2D convection-diffusion type operator is discretized with the help of second order upwind discretizations. The properties of smoothers are analyzed with Fourier two-grid analysis. Numerical solutions obtained for the option pricing problem are compared with reference results.

Key Words.
linear complementarity problems, American-style options, nonlinear multigrid, projected Gauss-Seidel, iterant recombination, second-order upwind discretization, Fourier analysis.

AMS(MOS) Subject Classifications.
65M55, 65F99, 90A09

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Forward References.

186 Towards robust 3D Z-pinch simulations: discretization and fast solvers for magnetic diffusion in heterogeneous conductors. *Pavel B. Bochev, Jonathan J. Hu, Allen C. Robinson and Raymond S. Tuminaro.*

Abstract.
The mathematical model of the Z-pinch is comprised of many interacting components. One of these components is magnetic diffusion in highly heterogeneous media. In this paper we discuss finite element approximations and fast solution algorithms for this component, as represented by the eddy current equations. Our emphasis is on discretizations that match the physics of the magnetic diffusion process in heterogeneous media in order to enable reliable and robust simulations for even relatively coarse grids. We present an approach based on the use of exact sequences of finite element spaces defined with respect to unstructured hexahedral grids. This leads to algorithms that effectively capture the physics of magnetic diffusion. For the efficient solution of the ensuing linear systems, we consider an algebraic multigrid method that appropriately handles the nullspace structure of the discretization matrices.

Key Words.
Maxwell's equations, eddy currents, De Rham complex, finite elements, AMG.

AMS(MOS) Subject Classifications.
76D05, 76D07, 65F10, 65F30

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vol.15.2003/pp186-210.dir/pp186-210.ps;
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Forward References.

211 Factors involved in the performance of computations on Beowulf clusters. *Paul A. Farrell and Hong Ong.*

Abstract.
Beowulf (PC) clusters represent ve platform for large scale scientific computations. In this paper, we discuss the effects of some possible configuration, hardware, and software choices on the communications latency and throughput attainable, and the consequent impact on scalability and performance of codes. We compare performance currently attainable using Gigabit Ethernet with that of Fast Ethernet. We

discuss the effects of various versions of the Linux kernel, and approaches to tuning it to improve TCP/IP performance. We comment on the relative performance of LAM, MPICH, and MVICH on a Linux cluster connected by a Gigabit Ethernet network. Since LAM and MPICH use the TCP/IP socket interface for communicating messages, it is critical to have high TCP/IP performance for these to give satisfactory results. Despite many efforts to improve TCP/IP performance, the performance graphs presented here indicate that the overhead incurred in protocol stack processing is still high. We discuss the Virtual Interface Architecture (VIA) which is intended to provide low latency, high bandwidth message-passing between user processes. Developments such as the VIA-based MPI implementation MVICH can improve communication throughput and thus give the promise of enabling distributed applications to improve performance. Finally we present some examples of how these various choices can impact the performance of an example multigrid code.

Key Words.
cluster computation, gigabit ethernet, TCP/IP performance, virtual interface architecture (VIA), MPI, MPICH, LAM, MVICH, NAS multigrid benchmarks.

AMS(MOS) Subject Classifications.
65Y05, 68M14, 68M12, 68M20, 68N99, 65Y20

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